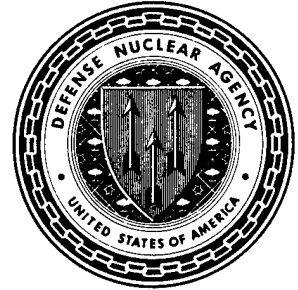




**Defense Nuclear Agency
Alexandria, VA 22310-3398**



DNA-TR-95-36

Numerical Methods for Nonclassical Gas Dynamics Involving Multi-Phase, Reactive Flows

**Harland Glaz
University of Maryland
Department of Mathematics
College Park, MD 20742**

February 1996

Technical Report

CONTRACT No. DNA 001-91-C-0095

**Approved for public release;
distribution is unlimited.**

19960129 077

DTIC QUALITY INSPECTED 1

Destroy this report when it is no longer needed. Do not return to sender.

PLEASE NOTIFY THE DEFENSE NUCLEAR AGENCY,
ATTN: CSTI, 6801 TELEGRAPH ROAD, ALEXANDRIA, VA
22310-3398, IF YOUR ADDRESS IS INCORRECT, IF YOU
WISH IT DELETED FROM THE DISTRIBUTION LIST, OR
IF THE ADDRESSEE IS NO LONGER EMPLOYED BY YOUR
ORGANIZATION.



DISTRIBUTION LIST UPDATE

This mailer is provided to enable DNA to maintain current distribution lists for reports. (We would appreciate your providing the requested information.)

- ☐ Add the individual listed to your distribution list.
- ☐ Delete the cited organization/individual.
- ☐ Change of address.

NOTE:

Please return the mailing label from the document so that any additions, changes, corrections or deletions can be made easily. For distribution cancellation or more information call DNA/IMAS (703) 325-1036.

NAME: _____

ORGANIZATION: _____

OLD ADDRESS

CURRENT ADDRESS

TELEPHONE NUMBER: () _____

DNA PUBLICATION NUMBER/TITLE

CHANGES/DELETIONS/ADDITIONS, etc.) (Attach Sheet if more Space is Required)

DNA OR OTHER GOVERNMENT CONTRACT NUMBER: _____

CERTIFICATION OF NEED-TO-KNOW BY GOVERNMENT SPONSOR (if other than DNA):

SPONSORING ORGANIZATION: _____

CONTRACTING OFFICER OR REPRESENTATIVE: _____

SIGNATURE: _____

CUT HERE AND RETURN



DEFENSE NUCLEAR AGENCY
ATTN: TITL
6801 TELEGRAPH ROAD
ALEXANDRIA, VA 22310-3398

DEFENSE NUCLEAR AGENCY
ATTN: TITL
6801 TELEGRAPH ROAD
ALEXANDRIA, VA 22310-3398

REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.				
1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE 960201	3. REPORT TYPE AND DATES COVERED Technical 911001-941231		
4. TITLE AND SUBTITLE Numerical Methods for Nonclassical Gas Dynamics Involving Multi-Phase, Reactive Flows		5. FUNDING NUMBERS C - DNA 001-91-C-0095 PE - 62715H PR - RA TA - RG WU - DH313770		
6. AUTHOR(S) Harland Glaz				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) University of Maryland Department of Mathematics College Park, MD 20742		8. PERFORMING ORGANIZATION REPORT NUMBER		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Defence Nuclear Agency 6801 Telegraph Road Alexandria, VA 22310-3398 TAIC/Rohr		10. SPONSORING/MONITORING AGENCY REPORT NUMBER DNA-TR-95-36		
11. SUPPLEMENTARY NOTES This work was sponsored by the Defence Nuclear Agency under RDT&E RMC Code B4662D RA RG 00260 400A AC 25904D.				
12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for Public release; distribution if unlimited.			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) This report documents recent progress in the field of numerical analysis of problems in fluid mechanics. The modeling equations include gas dynamics, incompressible flow, their viscous extensions, reactive flow and multiphase flow. Applications of these advanced methods in the areas of modeling blast wave environments and shock loading of nonclassical materials are discussed. New algorithms for problems involving coupled wave speed and source term stiffness, along with improved versions of multi-material extensions of the underlying compressible algorithm are discussed.				
14. SUBJECT TERMS Cloud Rise Shock Waves Conservation Laws Gas Dynamics Dusty Gases			15. NUMBER OF PAGES 22	
			16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT SAR	

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE

CLASSIFIED BY:

N/A since Unclassified.

DECLASSIFY ON:

N/A since Unclassified.

SECURITY CLASSIFICATION OF THIS PAGE

TABLE OF CONTENTS

Section	Page
1 INTRODUCTION	1
1.1 Implicit-Explicit Schemes	1
1.1.1 Zero Mach Number Limit	2
1.1.2 Chemically Reacting and Dusty Gas Flows	6
1.2 NonClassical Gas Dynamics	8
1.2.1 Nonconvex EOS	8
1.2.2 Multimaterial Algorithms	9
1.3 Incompressible Flows and the Projection Method	10
2 CONCLUSIONS	12
3 RECOMMENDATIONS	13
4 REFERENCES	14

SECTION 1

INTRODUCTION

The prediction of blast wave environments via numerical simulation is one of the organizing themes of the work discussed here and its original motivation. Such environments can be categorized as ideal or nonideal, as well as early time (equivalently, high overpressure) or late time (equivalently, low overpressure). The work reported on here is largely based on code technology developed in our preceding efforts at modeling high overpressure environments, both ideal and nonideal (using thermal layer models) [17]. Our code development efforts over the past few years have been directed at extending this technology in the following directions: (1) problems involving wave number stiffness which include as a special case nearly incompressible flow, (2) problems for which the incompressible equations themselves is appropriate, (3) problems involving source term stiffness and (4) problems involving strong shock wave propagation in materials with complicated constitutive properties. The applications which have focused this work arise largely from very late time blast wave environments, especially the problems inherent in the calculation of fireball rise. The motivation for our work in area (4) above comes, instead, from a desire to understand the effects of high overpressure blast waves on, for example, hardened targets or differing soil types.

If one considers the problem of fireball rise, it is immediately apparent that the analogue computational problem is really at least three problems: its initial formation, a long intermediate stage in which it begins to rise from a nearly stationary position and a late stage in which the local Mach number gradually increases and compressibility effects are once again important. For our purposes here, we consider the first part as solved by our older work. The second stage can be solved either by considering an incompressible model and solving the derived equations or by developing specialized implicit strategies in the context of a compressible flow solver. There is a stronger requirement for the latter approach as the Mach number increases at later times. On the other hand, related problems such as the prediction of contaminant transport in a battlefield or theatre environment are better handled by using an appropriate model with sonic waves eliminated a priori. Accordingly, we have worked on both approaches. At the same time, we have especially concentrated on particulate transport and reactive flow in these flow fields, since they are critically important inputs (and outputs) for the intended applications. This has led to our work on source term stiffness.

1.1 IMPLICIT-EXPLICIT SCHEMES.

In our report [17], we discussed the early stages of the development of the Implicit-Explicit (I-E) scheme, in particular some one-dimensional inviscid and viscous flow calculations, see [10]–[11], and we also presented future tasks. Several studies have been completed since and they represent major advances in this area. We start with a brief description of these studies. First, Collins has successfully accomplished several objectives that extended the generic I-E methodology; these were documented in great detail in his Ph.D dissertation [12]. Some aspects of this work were presented at the First European Computational Fluid Dynamics conference, see [14]. A summary of the objectives and results of the work carried out by Collins [12] and Collins et. al. [14] are given in Section 1.1.1 below. Second, the I-E methodology was implemented for flows that are modeled by systems with source terms, in particular chemically reacting and dusty gas models, including the cases of stiff sources, see [19] and [22]. The results of these studies are summarized in Section 1.1.2. below. Third, an early version of the work by Collins et. al (in the context of 1D flows) was submitted to and accepted for publication recently [13].

1.1.1 Zero Mach Number Limit.

The main objective of the work done by Collins [12] and Collins et al [13][14] is to eliminate the explicit Courant-Friedrichs-Levy (CFL) constraint on unsteady compressible flow calculations by using a high resolution explicit scheme in conjunction with an implicit scheme in such a way that the explicit CFL restriction is mitigated and that the solution retains much of the temporal accuracy provided by the explicit scheme. Explosion dynamics provides a particularly challenging example where this methodology is needed. There are two phases of interest in these types of problems: the initial blast wave and the subsequent cloud rise. Typically, the blast wave phase is computed using a high resolution explicit compressible code while the cloud rise is simulated with an incompressible code. At late time during the cloud rise phase, the Mach number becomes significant once again and can approach one; thus violating the assumption of incompressibility. The I-E strategy could be used to handle both phases of the problem, and in addition, it offers significant savings for just the blast phase of this problem. For example, if the temperature in the fireball is too high and the explicit time step of such calculation becomes too small for such calculation to be feasible, the scheme would allow for a much larger time step without significant degradation in the solution. At late times, the same code can be used to compute the cloud rise. As the Mach number in the cloud increases, the I-E method will transition continuously to a high resolution explicit scheme.

The study followed the guidelines stated below:

- (1) Develop an Eulerian implicit-explicit scheme, similar to the one in reference [16], which satisfies several design principles (for details, see, e.g., [14]).
- (2) Use the second-order Godunov scheme as the underlying high resolution explicit scheme.

- (3) Extend this method to two space dimensions using the unsplit Godunov scheme in [7].
- (4) Provide numerical calculations which demonstrate the feasibility of this method.

The work consists of two parts. In Part I, the method is implemented for the special case of one-dimensional inviscid compressible flow where, for convenience, a polytropic equation-of-state is used. The methodology can be easily extended to gas dynamics with a general equation-of-state using the ideas in [8]. A more difficult question is the extension of these ideas to two or three space dimensions; this was done in Part II for the two-dimensional case. Implementations for systems in higher space dimensions follows directly from the two-dimensional case.

At first, the implicit-explicit ideas are developed for the special case of linear advection in one space dimension; extensions of this linear scalar scheme to handle source terms follows. In particular, it is shown that this scheme satisfies the design principles, thereby fixing these ideas for extension to nonlinear systems. Also, the potential for nonlinear instabilities is recognized and an indication is given as to how to handle such instabilities. A nonlinear stability constraint is introduced for the method in the special case of a scalar conservation law. Next, the scheme is described for systems of conservation laws; the formulae necessary for compressible gas dynamics are included. For that case, it is assumed that a sufficiently smooth numerical flux function exists. Since Newton's method is used to solve the system in one space dimension, a key component of the work in Part I is the introduction of an appropriately smooth numerical flux function for the hyperbolic equations. A suitable version of the Engquist-Osher flux [6] is used, as modified for systems by Bell *et. al.* [4]. The version used is sufficiently smooth so that the Newton's method linearization is well-behaved; in particular, it converges to steady states even in the presence of strong shocks. The construction of this flux function, together with several approximations that are efficient for practical large-scale applications are presented in detail. For the two-dimensional system, an approximation to the Godunov flux is used and a nonlinear multigrid technique is applied to solve the resulting equations. To conclude the first part, numerical results are presented for the one-dimensional case. It is shown that the schemes are able to propagate slowly moving shocks and contact surfaces through a Cartesian mesh. Also, the scheme's ability to capture a stationary shock in a diverging duct is demonstrated. A numerical study is presented which demonstrates second-order accurate steady states.

In Part II, the scheme is generalized to two dimensions using Colella's Corner Transport Upwind (CTU) scheme [7] as the underlying explicit scheme. Once again, the focus is on the scalar linear advection equation, but this time in two space dimensions. The stability results here are far different from the one-dimensional case. The scheme of choice, i.e., the one studied in Part I, is unstable when applied to the scalar linear advection in two dimensions; therefore, in an effort to find a

better implicit scheme, a two parameter family of schemes is considered, with the same simple structure as the implicit scheme in Part I. A stable scheme is found but continuity in CFL number is lost. It is shown that even the stable implicit scheme is unstable when applied to the scalar linear advection equation in a hybrid mode. Because of this, the focus of attention shifts to the nearly incompressible flow application under the constraints that the particle characteristics are always handled explicitly (that is the advection part of the flow) whereas only the acoustic modes are treated implicitly.

Next, the truncation error and stability properties of the hybrid schemes are investigated, as applied to a linear system derived from the isentropic gas dynamic condition equations. The analysis is done under the assumption of nearly incompressible flow. The stability analysis indicates that, under not very restrictive constraints on the advection part of the flow, the original scheme is stable. Very similar results are obtained with the unconditionally stable implicit scheme discussed earlier. The truncation error analysis verifies the order of accuracy for the hybrid scheme, and in particular, verifies second order accurate steady states. It also shows why one cannot expect the scheme to work at arbitrarily low Mach numbers, problem for all compressible codes [29].

Part II is concluded with a presentation of computational results for two problems: a doubly periodic shear layer and a simulation of one of the Brown and Roshko shear layer experiments [5]. Both of these are examples of unstable, nearly incompressible flow. These results show that the scheme performs as desired; however, the efficiency of the nonlinear multigrid algorithm used in this study (and described in detail in [14]) leaves room for improvement.

To summarize this work we examine the results. The results of the 1D cases show that explicit high resolution upwind schemes can be smoothly hybridized on a mode-by-mode basis with an implicit method so that problems involving localized wave speed stiffness and convergence to steady state can be solved without sacrificing accuracy and resolution for strong wave interactions and energy containing modes. Several of the calculations illustrate the importance of replacing the Godunov flux by the smoother approximate Engquist-Osher flux when the system is linearized. Questions involving the optimal choice of an approximate Riemann solver and appropriate dissipative mechanisms have not been completely resolved; however, a very simple and efficient solver augmented by a small amount of artificial viscosity and some additional dissipation at sonic points has been capable of handling our test problems.

The stability results for this methodology in two space dimensions forced us to focus Part II on the low speed nearly incompressible flow application. The computational results for this part demonstrate that the implicit-explicit methodology is well suited for this application. The results show that for low Mach number flows, the degradation of the solution due to the implicit part of the computation

is minimal and the high resolution capability of the underlying explicit scheme is preserved. Also, since both the implicit and explicit results compare well with the incompressible results reported in reference [3], the approximate phase space solution and the Godunov flux discussed in detail in [14] appear to be adequate. The major drawback with the present implementation of this scheme is the cost of solving the nonlinear system. For the current multigrid implementation, calculations must be executed at a Courant number of approximately 7 or higher to be competitive with the explicit scheme; this corresponds to Mach numbers of 0.1 or lower. However, $M_\infty \leq .1$, it is questionable which solution strategy is competitive with the explicit code.

We remark that an attempt was made to accelerate the convergence of the resulting nonlinear system of equations by following the preconditioning matrix idea of Shuen et al [27]. This idea consists of introducing an extra derivative with respect to some pseudo-time; this additional finite difference derivative is premultiplied by preconditioning matrix and in the limit of steady-state with respect to pseudo-time the solution to the new system converges to the solution of the original (real) time-dependent system. The implicit-explicit method was rewritten following the methodology of [27] with the hope that the preconditioning matrix would accelerate the overall convergence of the scheme. It turned out that this idea did not work well for the I-E scheme; not only the performance did not improve but for some runs it resulted in diverging solutions. This behavior may be attributed to two different reasons: first, the analysis of [27] is dependent upon the finite-difference operator and the results quoted in [27] do not carry over to the I-E algorithm automatically, and second, it is not at all clear that the idea should improve time-dependent solutions in the first place; it is proven to work well for steady-state solutions but there does not exist enough evidence that the acceleration carries over to the time-dependent solutions.

We expect that there are many possible applications of the I-E approach taken here. In some of them (e.g., nearly incompressible flow) an obvious competing approach is to resolve the stiffness problem at the level of the governing equations by deriving a new system, asymptotically valid in the appropriate limit, which is not stiff and developing numerical methods for the limit system (e.g., the incompressible Euler equations). However, it should be noted that it is not known whether or not this approach is valid in all situations; for example, in the case of magnetohydrodynamics in the limit as the Alfvén number approaches zero, it does not appear to be possible to derive a limiting set of equations, see [18]. Also, it is usually more natural to derive well-posed initial-boundary value problems and design numerical boundary conditions for the original set of equations than for the reduced set in the appropriate approximation. Another class of problems for which our approach is an obvious candidate arises in atmospheric flows. Here, in addition to the Mach number varying widely, low amplitude gravity waves are present and restrict the time step considerably; eliminating the sound waves through the implementation of reduced equation sets can lead to numerical difficulties in specifying open boundary conditions.

The application of shock wave – boundary layer interaction, which we were not concerned with in this study, requires the hybrid scheme to transition from a fully explicit scheme in the free stream, to a hybrid scheme at the top of the boundary layer and possibly to a fully implicit scheme close to the wall. The stability results in Part II indicate that the transition to a fully implicit scheme in a two dimensional flow may lead to instabilities. These instabilities may never arise in this application for the following reasons: the flow in the boundary layer near the wall is essentially one-dimensional and from the analysis we know the flow has to be fully two dimensional for the instabilities to occur; and it may be the case that the viscous terms stabilize the scheme in this region. We have performed preliminary calculations using a viscous extension of the 1-dimensional method from Part I and directional operator splitting for shock wave – boundary layer interactions; the results indicate that our approach will be useful in this context. The implementation of a viscous extension of the unsplit code from Part II will be a topic for future work.

1.1.2 Chemically Reacting and Dusty Gas Flows.

The objective of this research effort is the efficient and accurate computation of reactive multiphase flows at both high and low Mach numbers (e.g., boundary layers, combustion, among others). We believe that the I-E strategy, when coupled with mesh refinement approaches and methods for the stable computation of stiff source terms, can be a valuable tool in this field. We start with the description of preliminary study reported in [19].

The purpose of the study in [19] was to further advance and validate the I-E approach by investigating the effects of including source terms representing multispecies reacting flows. The integration scheme for the sources was done either fully explicit or using the trapezoidal rule, but in both cases the sources were not projected onto left and right states in the setup of initial data for the flux function approximation (or Riemann problem). Several 1D results were obtained; converged solutions for variable area duct, for both smooth and shocked flows are demonstrated using an extension of the Newton iteration methodology of Collins et al [14]. Also, an appropriate extension of the unsplit I-E scheme has been developed and implemented for 2D reactive flow with periodic boundary conditions; the new scheme was used for problems analogous to the nonreactive results discussed above for the zero Mach number limit.

For the 1D calculations we find that the performance criteria depend on the degree of source term stiffness. In particular, a fairly low CFL maximum is required (that is, to obtain converged solutions) during parts of the calculations. Unlike the 1D calculations, it is found that trapezoidal rule differencing for the source terms is required for stability for the 2D problem solved. In view of these results we decided to explore more complex treatments of stiff source terms and, especially, the coupling between wave speed and source term stiffness. These issues were addressed in the work reported in [22] and described next.

The work discussed here is concerned with the problem of source-term stiffness which arises in, e.g., reactive flow and/or two-phase flow. We studied several new innovative approaches due to Yee et al [23] [25] [30], Pember [26] and the present authors. Several ideas were then applied in the context of the Godunov-like, hybrid implicit-explicit scheme so that the latter methodology was successfully extended to treat both stiff and non-stiff, nonequilibrium, chemically reacting flow fields. This is done using a completely unsplit operator: both the two-dimensional and the source terms integrations are fully coupled. For the fully explicit mode of the scheme, the procedure used allows for the formal retention of second-order accuracy of the numerical scheme.

The stiff and nonstiff solvers developed here were used to solve two unsteady flow cases: a doubly periodic, unstable, low Mach number shear layer flow and the simulation of the evolution of a shock wave due to the transverse injection of fluid into supersonic flow. In both flow fields, and for several reaction models (i.e., frozen air flow, air with only vibrational relaxation of molecules and a complete chemically reacting, 5-species air model), the numerical results prove that the extended implicit-explicit methodology can handle complex flow problems and compute high-resolution details. We found that the standard non-stiff approach cannot handle stiff problems; even upon starting up with very small integration steps, the solution becomes unstable and eventually breaks down.

We have also shown via numerical experimentation that after the resolution of the initial large gradients in stiff flow fields, using the fully explicit mode of the solver, the solution remains stable in the neighborhood of the thermodynamical equilibrium state and can be advanced in time using the implicit-explicit mode; although the I-E mode does not theoretically provide the same order of accuracy, it may be used due to its relative efficiency. Therefore the stiff I-E solver can handle stiffness arising both from sources and wave speeds.

None of the above reports contain our work on dust modeling. The code described here contains most of the modules needed to model stiff dusty gas flows. Although similar in many respects to the problems of reactive flow, there are additional numerical difficulties which have been addressed in the course of our code development work. Future tasks are to optimize the code, specifically by searching for and implementing faster nonlinear solvers in the implicit modes of the predictor and the corrector steps (e.g., multigrid methodologies, see [12]). Also, the importance of the Riemann problem solver (and related numerical models) needs to be studied in conjunction with the solution of stiff, close-to-equilibrium thermodynamic states.

1.2 NONCLASSICAL GAS DYNAMICS.

1.2.1 Nonconvex EOS.

The motivation for the study of 2D unsteady isentropic gas dynamics (2×2 system) with a nonconvex equation of state (EOS), as well as the results of the work that was carried out during 1989-1991, are described in detail in [17], [20]. A brief summary of the main objectives follows: first, to simulate the α - ϵ phase transition in Iron which occurs at about 137 kilobars and has been extensively studied; second, to test several variants of the second-order Godunov scheme in the simple 2×2 setting, but for materials with nonconvex EOS.

The nature of the above mentioned study restricted us to using very particular nonconvex EOS's. We used two models. The first was obtained by using simple polytropic gas relations such as $p(v) = v^\gamma$, where p is the pressure, v is the specific volume, and γ is the ratio of specific heats, and joining two (locally) convex disjoint "pieces" of the above curve by adding a C_0^∞ function so that the resulting nonconvex EOS has two isolated zeroes in the second derivative and the function is monotonically decreasing. The second model was based on experimental data of the two distinct α - ϵ phases of Iron along the isotherm $T = 295^\circ$ K; since the EOS curves describing the two phases do not cross in the transition region, we carefully constructed a smooth joining (transition) curve which consists of a fifth order polynomial with second order contact at the end points. As a consequence, and for both models, the Riemann problem defined for any two initial states on the EOS curve has a unique solution, composed of both nonclassical and classical waves, that can be theoretically predicted (see, e.g., [28]) and numerically constructed; we point out that such solutions are complex, tedious to program and very expensive to compute exactly.

The results of the above mentioned work are given briefly here. First, we developed robust and accurate numerical schemes for the solution of problems described by 2×2 model equations with a nonconvex EOS; specifically, we found that the general methodology of Bell-Colella-Trangenstien (BCT) [4] yielded excellent quality results at acceptable expense compared to other Godunov-like schemes. Second, we conducted a limited study of self-similar, oblique shock wave reflections in two space dimensions. We have found new and quite exciting phenomenology resulting from the nonconvexity that induces highly nontrivial 2D wave interactions.

The work summarized above has been extended in two directions. First, we obtained more results in the 2×2 context; we used the BCT schemes to perform new calculations in which the EOS has a cusp. The latter seems to more realistically describe phase transitions compared to the smooth curves constructed for the transition region in our preceding work described above. The results are extremely interesting, especially for regular to Mach transition, and they clearly indicate the capturing of split waves as predicted by the theory for such EOS models. More runs and analysis are required for the better understanding of this phenomenon.

A summary of this ongoing work can be found in [21]. Second, and more importantly, we have extended the BCT algorithm to the full equations of gas dynamics (3×3 system). The current draft of E. Erskine's Masters thesis [15] contains the fundamental results necessary to extend the BCT algorithm to the 3×3 case and do realistic material modeling; some preliminary numerical results in 1-space dimension setting were presented by E. Erskine in April 1993 at a meeting in Stonybrook, NY. More advanced code development work for the 3×3 case took place in the last few months. A generic version of a BCT-like, split, two-spatial dimensions code was written and results for a convex strong shock reflection were obtained and compared with the solutions obtained using the "usual" second-order Godunov scheme; the comparison shows excellent agreement. Currently, several nonconvex EOS are being analytically constructed (a nontrivial issue for the 3×3 case where the nonconvexity is constructed in the energy equation under several thermodynamical constraints) and they will be tested in the two-dimensional, shock-reflection setting (some very early results are available). Also, we are surveying the literature for experimental data that could assist us in modeling realistic materials. We point out that the results for the nonconvex 3×3 case are new, it is not clear how the physical model translates into the reflection diagram and we believe that a large number of runs and exhaustive analysis will be required to verify the solutions and to have a good feel and understanding of the new phenomenon.

1.2.2 Multimaterial Algorithms.

For a description of the main issues and applications for multimaterial extensions of our codes see [17]. During the contract period, it became apparent that our method was failing for the case of a strong rarefaction in water. Consequently, considerable effort has gone into extending our analysis and fixing the code. This work is now complete as well as successful – at least for the Tait EOS. Details are available in the current draft of [9].

1.3 INCOMPRESSIBLE FLOWS AND THE PROJECTION METHOD.

The early development of the projection method is discussed in [17]. Since then, J. Bell and colleagues at LLNL worked at extending the code to treat variable density, 3-D flow fields and also combustion in the zero Mach number limit [24]. The development of a 3-D code with Adaptive Mesh Refinement (AMR) capabilities is ongoing at LLNL. After completion, it will be possible to use the latter to simulate the low speed part of fireball rise. In what follows we will describe some preliminary studies that were conducted with a non-AMR (i.e., uniform mesh), 2-D version of the code that was provided by D. Marcus (LLNL).

The idea is to numerically model the cloud rise experiments known as GEST (Gas Explosive Simulation Technique, see [3]–[4]) by first solving the explosion phase using a compressible flow solver and, after some appropriate evolution time, assuming that the residual flow field in the explosion vicinity is incompressible, carry out the solution of the cloud rise phase using an incompressible flow solver. We can proceed as follows. A spherical explosion was modeled incorporating the (1D) Godunov compressible code and using the input data produced by A. Kuhl (stoichiometric Methane–Oxygen mixture). The computation was carried out by us to the physical time $T = 1.0$ sec., for which the leading shock wave has already left the computational domain (and region of interest for the incompressible flow model). We remark that this part of the computation was done on a relatively fine (and uniform) mesh.

The output data obtained by the latter computation, in its conservative form, is used as input data for the second phase of the computation. First, the (spherical) one-dimensional conservative variables are mapped onto a two-dimensional, cylindrical (r - z) coordinate system; this is done by insisting that the variables remain conservative with respect to the new cell-volumes, created by the relatively coarse cylindrical mesh, and assigning the appropriate (i.e., volumetric) weight to the computed variables by tracing their fine-mesh-volume contributions to the new cells (in which they are fully contained or partially intersected). The incompressible flow model requires only the density and velocity fields. However, we also map the composition (i.e., product gas/air ratio) and simply “convect” this variable in the evolving incompressible flow field in order to extract temperature data from the local density and composition data.

As mentioned above, the incompressible solver we have at present is a non-AMR, 2D version of the second-order projection method. The computational domain chosen for the intended preliminary work consists of 256 by 512 zones, modeling a physical domain of 50m (r) by 100m (z). The initial data consists of a post-explosion sphere of radius of 30m mapped onto the cylindrical domain and centered at the point of ignition of the explosive device; the zones outside the sphere take on the ambient air conditions. The important underlying hypothesis of a divergence free velocity field for the incompressible flow model is (numerically) imposed on the initial data

at the beginning of the computation. In addition, we can code and compute the physical locations of the ten probes that recorded data in the live experiment, tag the (numerical) cells "containing" these probes, and record time-dependent data at these ten locations. Several other diagnostic data can also be recorded during the "cloud rise" computational phase. A complete run, one which advances the flow from $T = 1.0$ sec. (end of compressible flow solver) to about $T = 4.0$ sec. (the data recordings of the successful experiment terminated at about $T = 3.8$ sec.), is expected to take about 800 time steps at a cost of about one CPU hour on a Cray YMP.

The results would consist of the time dependent density, velocity, vorticity and composition fields. The vorticity field will capture the roll up of vortices and their motion upwards, based on previous work with this code technology. A full analysis of such a calculation must await the results. We are now completely prepared to proceed with this effort.

SECTION 2

CONCLUSIONS

- (1) The implicit-explicit methodology has been extended to near zero Mach number situations and accurate, resolved results have been computed. Source term capability – stiff and nonstiff – has been successfully implemented in the context of realistic physics modeling.
- (2) The variable density projection algorithm is a highly robust, accurate and efficient method for problems which are essentially zero Mach number at all times of interest, e.g., cloud rise. It is the method of choice for such situations.
- (3) The multimaterial algorithm is now available for water using the Tait EOS. More generally, the algorithm is now being used by many groups with great success.
- (4) It has been shown that materials characterized by nonclassical EOS exhibit solution phenomenology which can be profoundly different from convex EOS gases. The implications of this are quite profound for the numerical prediction of shock and blast wave loading; it is necessary that the underlying code integrator be capable of capturing all of the physically relevant waves **and** do so if and only if they are actually present in the mathematical solution.

SECTION 3 RECOMMENDATIONS

- (1) The implicit-explicit code remains one of two possibilities for computing problems with inherent wave speed stiffness, along with hybrids of projection codes and explicit upwind schemes. Further research is essential if endusers are to have confidence in the results from simulations of problems such as fireball rise where the Mach number can increase substantially during the course of the calculation.
- (2) The explicit codes for gas dynamics are now a fairly mature technology. Our research on multimaterial extensions and more complicated conservation laws leads to the conclusion that code development efforts in this direction would payoff in greatly improved predictive capabilities for applications such as blast wave loading of soil, reinforced targets, etc. and advanced HE weapon design (including interior ballistics).
- (3) The zero Mach number projection methodology is advancing rapidly and it appears that it's extension to long-time transport at large length scales (including mesoscale) will pose no theoretical difficulties. In view of the relatively low level of sophistication in the numerical modelling in currently available codes for this problem domain, a large effort here promises even larger payoffs.

REFERENCES

1. R. G. Batt, *Hot Wire Measurements of Temperature Field Structure Within GEST Fireballs*, Technical Report DNA 3936F.
2. R. G. Batt, R. A. Bigoni and D. J. Rowland, *Temperature-Field Structure Within Atmospheric Buoyant Thermals*, J. Fluid Mech. **141** (1984), 1-25.
3. J. B. Bell, P. Colella and H. M. Glaz, *A Second-Order Projection Method for the Incompressible Navier-Stokes Equations*, J. Comput. Phys. **85** (1989), 257-283.
4. J. B. Bell, P. Colella and J. A. Trangenstein, *Higher Order Godunov Methods for General Systems of Hyperbolic Conservation Laws*, J. Comput. Phys. **82** (1989), 362-397.
5. G. L. Brown and A. Roshko, *On Density Effects and Large Structure in Turbulent Mixing Layers*, J. Fluid Mech. **64** (1974), 775-816.
6. K.-Y. Chien, R. E. Ferguson, A. L. Kuhl, H. M. Glaz, & P. Colella, *Inviscid Simulations of Turbulent Shear Layers-Mean Flow Profiles*, In proceedings of the International Workshop on the Physics of Compressible Turbulent Mixing, Princeton University, Princeton, NJ, 24-27 October 1988. In press.
7. P. Colella, *Multidimensional Upwind Methods for Hyperbolic Conservation Laws*, J. Comp. Phys. **87** (1990), 171-200.
8. P. Colella and H. M. Glaz, *Efficient solution algorithms for the Riemann problem for real gases*, J. Comp. Phys. **59** (1985), 264-289.
9. P. Colella, H. M. Glaz and R. E. Ferguson, *Multifluid Algorithms for Eulerian Finite Difference Methods*, in preparation.
10. J. P. Collins, *An Implicit/Explicit Higher Order Godunov Scheme*, Naval Surface Warfare Center Rep. NSWC TR 88-320, 1989.
11. Collins, J. P., *Viscous Oblique Shock Reflections Using an Implicit/Explicit Higher Order Godunov Scheme*, Presented at the 9th International Mach Reflection Symposium, Ernst-Mach-Institut, Freiburg, FRG, 18-21 June, 1990.
12. Collins, J. P., *Implicit/Explicit Godunov Schemes for Unsteady Gas Dynamics*, Ph. D. Dissertation, University of Maryland at College Park, Department of Mathematics, 1992.
13. J. P. Collins, P. Colella and H. M. Glaz, *An Implicit-Explicit Eulerian Godunov Scheme for Compressible Flow*, J. Comput. Phys. in press.
14. Collins, J. P., Colella, P. and Glaz, H. M., *An Unsplit Implicit-Explicit Godunov Method for Compressible Gas Dynamics*, in Computational Fluid Dynamics 1992, Vol. II, pp. 659-666, Proc. First European CFD Conf., ed. Ch. Hirsch (Elsevier).
15. Erskine, E., *BCT Algorithm for 3×3 Gas Dynamics With a Nonconvex Equation of State*, in preparation.
16. B. A. Fryxell, P. R. Woodward, P. Colella and K. H. Winkler, *An Implicit-Explicit Hybrid Method for Lagrangian Hydrodynamics*, J. Comp. Phys. **63** (1986), 283-310.
17. H. M. Glaz, *Multiburst and Fracticide Effects. Task One: Numerical Methods and Computational Results*, DNA Report DNA-TR-90-199.
18. S. Klainerman and A. Majda, *Singular Limits of Quasilinear Hyperbolic Systems with Large Parameters and the Incompressible Limit of Compressible Fluids*, Comm. on Pure and Applied Math. **34** (1981), 481-523.
19. Krispin, J. and Glaz, H. M., *Nonequilibrium, Chemically reacting Flowfields and the Implicit-Explicit Godunov Scheme*, Proc. 13th International Conference on Numerical Methods in Fluid Dynamics, Rome, Italy 1992, eds. M. Napolitano and F. Sabetta, Springer-Verlag.
20. Krispin, J., Collins, J. P. and Glaz, H. M., *High-Order Godunov Type Solutions for Materials Having a Nonconvex Equation of State*, AIAA-91-1576, 1991.
21. Krispin, J., Collins, J. P. and Glaz, H. M., *High-Order Godunov Methods for Isentropic Gas Dynamics with a Nonconvex Equation-of-State*, in preparation.
22. Krispin, J., Glaz, H. M., and Collins, J. P., *High Resolution Solutions to Stiff Chemically Reacting Flows*, AIAA-94-0173, 1994.
23. A. Lafon and H. C. Yee, *On the Numerical Treatment of Nonlinear Source Terms in Reaction-Convection Equations*, AIAA-92-0419, 1992.

24. Lai, M. Bell, J. B., and Colella, P., *A Projection Method for Combustion in the Zero Mach Number Limit*, AIAA-93-3369-CP.
25. R. J. LeVeque and H. C. Yee, *A Study of Numerical Methods for Hyperbolic Conservation Laws with Stiff Source Terms*, NASA TM-100075, 1988.
26. Pember, R. B., *Numerical Methods for Hyperbolic Conservation Laws with Stiff Relaxation II. Higher Order Godunov Methods*, UCRL-JC-109097 Pt. 2.
27. J. -S. Shuen, K. -H. Chen and Y. Choi, *A Time-Accurate Algorithm for Chemical Non-Equilibrium Viscous Flows at All Speeds*, AIAA-92-3639, 1992.
28. B. Wendroff, *The Riemann Problem for Materials with Nonconvex Equations of state I : Isentropic Flow*, J. of Math. Anal. and Appl. **38** (1972), 454-466.
29. H. C. Yee, *A Class of High-Resolution Explicit and Implicit Shock-Capturing Methods*, NASA Technical Memorandum 101088, 1989.
30. H. C. Yee and J. L. Shinn, *Semi-Implicit and Fully Implicit Shock-Capturing Methods for Hyperbolic Conservation Laws with Stiff Source Terms*, AIAA-87-1116-CP, 1987.

DISTRIBUTION LIST

DNA-TR-95-36

DEPARTMENT OF DEFENSE

DEFENSE INTELLIGENCE AGENCY

ATTN: DIW-4

ATTN: RTS

DEFENSE NUCLEAR AGENCY

ATTN: RAST W SUMMA

ATTN: SPWE

2 CY ATTN: TSTL

DEFENSE TECHNICAL INFORMATION CENTER

2 CY ATTN: DTIC/OCF

FIELD COMMAND DEFENSE NUCLEAR AGENCY

ATTN: FCPR

ATTN: FCT COL H LAWSON

FIELD COMMAND DEFENSE NUCLEAR AGENCY

ATTN: FCTO

DEPARTMENT OF THE ARMY

ARMY RESEARCH LABORATORIES

ATTN: AMSRL-WT-NJ

DEP CH OF STAFF FOR OPS & PLANS

ATTN: DAMO-NCZ

U S ARMY SPACE STRATEGIC DEFENSE CMD

ATTN: CSSD-SA-E

USASSDC

ATTN: CSSD-H-SA

DEPARTMENT OF THE NAVY

DEPARTMENT OF THE NAVY

ATTN: CODE R44 H GLAZ

NAVAL RESEARCH LABORATORY

ATTN: CODE 5227 RESEARCH REPORT

OFFICE OF CHIEF NAVAL OPERATIONS

ATTN: NUC AFFAIRS & INT'L NEGOT BR

DEPARTMENT OF THE AIR FORCE

AIR UNIVERSITY LIBRARY

ATTN: AUL-LSE

WL/ELE BLDG 620

ATTN: WRDC/MLP

ATTN: WRDC/MTPM

DEPARTMENT OF ENERGY

LAWRENCE LIVERMORE NATIONAL LAB

ATTN: J CAROTHERS

ATTN: GOUDREAU

ATTN: P CHRZANOWSKI

ATTN: DR S J SACKETT

ATTN: G POMYKAL

SANDIA NATIONAL LABORATORIES

ATTN: J RIGALI 9800

OTHER GOVERNMENT

CENTRAL INTELLIGENCE AGENCY

ATTN: OSWR/NED 5S09 NHB

DEPARTMENT OF THE INTERIOR

ATTN: D RODDY

DEPARTMENT OF DEFENSE CONTRACTORS

AEROSPACE CORP

ATTN: H MIRELS

INFORMATION SCIENCE, INC

ATTN: W DUDZIAK

JAYCOR

ATTN: CYRUS P KNOWLES

KAMAN SCIENCES CORP

ATTN: D CAYNE

KAMAN SCIENCES CORPORATION

ATTN: DASIAK

MAXWELL LABORATORIES, INC

ATTN: J MURPHY

PACIFIC-SIERRA RESEARCH CORP

ATTN: H BRODE

SCIENCE APPLICATIONS INTL CORP

ATTN: H WILSON

SCIENCE APPLICATIONS INTL CORP

ATTN: R WESTERFELDT

SCIENCE APPLICATIONS INTL CORP

ATTN: J COCKAYNE

SCIENCE APPLICATIONS INTL CORP

ATTN: G BINNINGER

TRW INC

ATTN: TIC

TRW SPACE & DEFENSE SECTOR

ATTN: D M LAYTON

ATTN: W WAMPLER

UNIVERSITY OF MARYLAND

2 CY ATTN: H GLAZ

VITRO CORP

ATTN: H BRIGHT

WEIDLINGER ASSOCIATES, INC

ATTN: P WEIDLINGER